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TUNNELLING FROM NON-LOCALISED INITIAL STATES

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ABSTRACT

We present a new approach for calculating tunnelling amplitudes from a non-localised initial state. Generalising the matching conditions and equations of motion to allow for 'complex' momentum permits a description of tunnelling in the presence of so-called classical motion. We comment on possible applications of the method.

That quantum mechanical probability density can permeate into regions in which a classical particle is forbidden was (and perhaps still is) one of the more intriguing features of the Schrödinger equation. Rapidly however, it was turned into one of the major successes of the early wave mechanics in providing a successful theoretical description of alpha particle emission in radioactive decay. Since then, tunnelling has found many applications, yet our understanding of many aspects of the phenomenon remains limited. Motivated by difficulties[1] in calculating tunnelling amplitudes in recent two-field inflationary models[2-4], we re-examined the quasi-classical approximation to the Schrödinger equation to see if one could incorporate more complicated evolution of the wave function without losing the simplicity of that approach. We found that the problem reduces to two key issues: that of incorporating complex momentum into a quasi-classical description, and the related problem of matching conditions between different asymptotic régimes. Here we will show how to resolve these questions, illustrating some results from a test potential. A more detailed exposition may be found in a companion paper[5].

First let us summarise the current status for calculating tunnelling amplitudes. Most tunnelling calculations proceed via the quasi-classical approximation[6], which extracts the leading order "classical" behaviour of the system. If we assume the wave function takes the form

$$\Psi(\mathbf{x}, t) = e^{i\sigma(\mathbf{x})/\hbar} e^{-iEt/\hbar} , \qquad (1)$$

then the Schrödinger equation gives

$$\frac{1}{2m}(\nabla\sigma)^2 - \frac{i\hbar}{2m}\nabla^2\sigma = E - U(\mathbf{x}) \qquad (2)$$

as the equation of motion for σ. The quasi-classical approximation drops the $O(\hbar)$ term in (2), which clearly requires that $|\nabla\sigma|^2 \gg \hbar|\nabla^2\sigma|$.

In tunnelling, we need to solve the Schrödinger equation in regions where $U > E$, therefore we set $\sigma = ig$ and obtain

$$(\nabla g)^2 = 2m(U - E) \qquad (3a)$$

$$\Rightarrow \qquad g = \int^{x_f} \sqrt{2m(U - E)}dl, \qquad (3b)$$

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where l is the path which minimises the integral and x_f is the point of emergence of that path into the classical régime. This geometric solution to the problem in more than one dimension was first obtained by Banks, Bender and Wu[7] for the case of tunnelling from a localised state, they called l the *escape path*. The calculation of l and g in practise is facilitated by the Euclidean time prescription whereby we associate ∇g with $\mathbf{p}_e$, a Euclidean momentum, and (3a) becomes a Hamiltonian problem of particle motion in the (inverted) potential $-U$. It is then a classical dynamics problem to calculate the trajectory $\mathbf{x}(\tau)$, which interpolates between the initial position and the position of emergence from the barrier.

This approach is powerful, however it does have one crucial restriction, namely, it requires that space be divided into regions in which $\nabla\sigma$ is entirely real or entirely imaginary so that we can identify $\mathbf{p} = \nabla\sigma$ with some $\dot{\mathbf{x}}$("time"). Clearly we then need $\dot{\mathbf{x}}$ to vanish on the boundaries between these regions. In the context of the escape path, we need $\dot{\mathbf{x}}^2 \to 0$ at each end of the path. In general it requires two initial conditions to fix the start of the escape path, which uses up the requisite number of boundary conditions, leaving no additional freedom for the end point, which in general will not satisfy $\dot{\mathbf{x}}^2 = 0$. Another related problem is that we have no allowance for the transport of real momentum under a barrier, which we know definitely does occur in the case of a continuous symmetry. There is also the problem of picking an initial position from which to integrate, since we can only localise a particle at the expense of information about its momentum. We clearly need a more general picture of tunnelling.

In order to solve the Schrödinger equation when the momentum is complex, we rewrite (2) in terms of the real variables f and g, where $\sigma = f + ig$:

$$(\nabla f)^2 - (\nabla g)^2 + \hbar\nabla^2 g = 2m(E - U) \qquad (4a)$$

$$2\nabla f.\nabla g - \hbar\nabla^2 f = 0. \qquad (4b)$$

In the quasi-classical approximation we neglect the $O(\hbar)$ terms in these equations, this will be valid unless

$$(\nabla f)^2 \sim \hbar\nabla^2 f$$
$$(\nabla g)^2 \sim \hbar\nabla^2 g \qquad (5)$$

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i.e. unless $|\nabla f|$, $|\nabla g|$ is small or $|\nabla^2 f|$, $|\nabla^2 g|$ large, this latter situation occurs at caustics of the motion. The simplest way to visualise this is to consider a plane wave scattering off some barrier. The integral curves of ∇f trace out the path that a family of classical particles would follow in that potential. Clearly, neighbouring, initially parallel, trajectories will at some stage cross, and at such a place, referred to as a caustic, $\nabla^2 f$ becomes unbounded.

Having identified the boundary between different asymptotic regions, we now focus on the turning surface to obtain the matching conditions. We first consider a local coordinate system along the caustic $\{x, y^i\}$ where x is orthogonal distance from the caustic, and the y^i are cartesian coordinates in the surface of the caustic. Provided the caustic is not too strongly curved, the potential is roughly a function of x, and we may deduce that the true (continuous) solution of the Schrödinger equation is

$$\psi(x, y^i) = e^{ip_i y^i/\hbar} \text{Ai} \left(\hbar^{-2/3} (2mU_{,x})^{1/3} \left[x + \frac{E - U(0) - \frac{p_i^2}{2m}}{U_{,x}} \right] \right) \qquad (6)$$

where $\text{Ai}(x)$ is the Airy function. That the curvature of the caustic not be too large translates to a bound on $\nabla_i^2 U$: noting that (6) implies that the quasi-classical approximation breaks down when $|x| \leq \hbar^{2/3}(2mU_{,x})^{-1/3}$, we obtain a limit of $\nabla_i^2 U \ll \hbar^{-4/3} U_{,x}^{2/3}$. Equation (6) gives us the inital conditions for f and g for integrating out beyond the caustic. Clearly the parallel momenta, p_i are conserved across the boundary, i.e. $\nabla_i f$, $\nabla_i g$ conserved. The orthogonal components are determined on either side of the boundary by using equation (4a) and demanding that real (∇f) and imaginary (∇g) momenta be orthogonal (equation(4b)). This fixes the initial conditions for the momentum on the other side of the boundary. We now need to propagate f and g out from the boundary, i.e. solve (4a,b).

In order to facilitate the solution of (4a) we assume $E \ll U$, which implies that ∇g is dominant under the barrier, however, we do not wish to neglect ∇f as an $O(\hbar)$ correction, otherwise we would use existing techniques. Instead we want to consider a situation where $\hbar \ll \frac{E}{U} \ll 1$, and iteratively solve

$$(\nabla g)^2 = 2mU - (2mE - (\nabla f)^2) \qquad (7a)$$

$$\nabla f . \nabla g = 0, \qquad (7b)$$

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bearing in mind that $(\nabla f)^2$, E are of the same order, and small compared with $(\nabla g)^2$, U.

The first step is to find the leading behaviour, that is, to solve $(\nabla g)^2 = 2mU$. In order to do this, we use existing techniques. We regard the solution under the barrier as being composed of a family of escape paths $\{l_{(\alpha)}\}$ originating from the turning surface at $(y^i_{(\alpha)}, 0)$, and propagating under the barrier until a caustic is reached. Along each escape path we have a solution for g determined by (3b) with $E = 0$. This will give us a leading order solution to the problem. Now we use the information from (7b), that f is constant along integral curves of g, to set $f = f(\varphi^i_{(\alpha)}(\mathbf{x}))$ where $\varphi^i_{(\alpha)}(\mathbf{x}) = y^i_{(\alpha)}$ are the equations for the family of escape paths $l_{(\alpha)}$. Finally, we input this solution for f back into (7a) to obtain the correct form of g to order E/U. Once we have the solution under the barrier we may match across into the far 'classical' régime and follow a similar procedure to the above to complete the solution of the Schrödinger equation.

To recap: this method solves the Schrödinger equation in the stationary quasi-classical approximation for tunnelling in potentials with non-localised minima. The restrictions on the type of potentials it can deal with are that $E \ll U$ under the barrier and that the transverse derivatives of U at the matching boundary be bounded by $\hbar^{-4/3} U_{,x}^{2/3}$. This method is therefore ideal for problems involving scattering off a 'wall'.

As a simple illustration of the method, consider a plane wave, $e^{i\mathbf{k}\cdot\mathbf{x}/\hbar}$, scattering off a wedge potential in two dimensions, $U(\mathbf{x}) = V\Theta(x)\Theta(a - x - \epsilon y)$, see fig. 1. Here, our initial conditions at $x = 0$ are $g = 0$, $f = k_2 y_i$, $g_{,x} = \sqrt{2mV}$ and $f_{,x} = 0$. Integrating out is straightforward since the potential is constant and gives $g = \sqrt{2mV}x$. Imposing $f = $const. along integral curves of g, which in this case are $y = y_i$, simply gives $f = k_2 y$, then inputting this back into (7a) gives $g = \sqrt{2mV - k_1^2}x = \kappa x$. In this example our iterative procedure under the barrier is now complete. At the far edge of the barrier the appropriate boundary conditions are now non-standard, the momentum parallel to the far edge being complex: $p_\parallel = (p_2 - i\epsilon\kappa)\mathbf{T}$, where $\mathbf{T}$ is the tangent vector to the far edge of the barrier. Orthogonality of the real and imaginary momenta and (7a) requires that $p_\perp = (p_1 + i\epsilon\kappa\frac{p_2}{p_1})\mathbf{N} + O(\epsilon^2)$. Setting

$$\xi = x - a + \epsilon y \quad , \quad \eta = y - \epsilon(x - a) \tag{8}$$

(see fig. 2) we may integrate out from the boundary to obtain

$$f_{out} = p_1 \xi + p_2 \eta$$

$$g_{out} = \kappa a - \epsilon \kappa \eta + \frac{p_2}{p_1} \epsilon \kappa \xi \tag{9}$$

Note some interesting features about this solution. The incoming and outgoing real momenta are not parallel, although they subtend the same angle with each side of the barrier. Note too that g is spatially dependent, decreasing in regions where the barrier is thinner. However, the really curious features of scattering off this potential are most clearly exhibited if we consider a Gaussian wave packet scattering off the barrier. For the sake of definiteness we take the momentum to be peaked at (p_1, p_2) with spread $\lambda \hbar^2$, hitting the origin at $t = 0$. Such an incident wave packet might reasonably be supposed to represent a particle scattering off the barrier. For the trajectory of the outgoing peak we obtain

$$\eta = \frac{p_1 \xi}{p_2(1 - 2a\lambda\hbar/\kappa)} + \frac{\epsilon\kappa}{2\lambda\hbar} \left(1 + \frac{p_2^2}{p_1^2}(1 - 2a\lambda\hbar/\kappa)^3 \right) \tag{10}$$

with a transmission amplitude of $e^{-\kappa x_{out}/\hbar}$. In other words, a particle 'incident' on the barrier at $t = x = y = 0$ emerges at $\eta_e = \frac{\epsilon\kappa}{2\lambda\hbar}(1 + \frac{p_2^2}{p_1^2}(1 - 2a\lambda\hbar/\kappa)^3)$. One can also calculate the time of emergence, $t_e = \frac{m\epsilon\kappa p_2}{2\lambda\hbar p_1^2}(1 - 2a\lambda\hbar/\kappa)^3$. The particle emerges considerably 'downstream' from where one might expect it, neither at $x = (a, 0)$, nor at $x = (a, \epsilon a)$, but at $x = (a - \epsilon\eta_e, \eta_e)$. Furthermore, the time at which it emerges is potentially large compared with $\hbar$ and even, if $p_2 < 0$, potentially negative! In fact, both these peculiarities arise from a simple physical reason, the fact that the most energetically favourable time for the Gaussian to tunnel is not necessarily when the peak hits the barrier. Tunnelling amplitudes depend exponentially on the size of the barrier, therefore it is more favourable to tunnel where the barrier is thinner, hence the dependence of the transition amplitude on x_{out}. On the other hand, the probability density along $x = 0$ is damped by an exponential factor depending upon how far away that point is from the peak of the Gaussian. Clearly there will be a pay off between these two factors which *may* mean that it is more energetically favourable for the fringe of the Gaussian to tunnel, rather than its peak.

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Apart from giving an initial step in the problem of calculating two-field tunnelling amplitudes, our method (and illustrative example) may also have applications in other areas of tunnelling theory. For instance, one of the outstanding problems in tunnelling is defining a unanimously acceptable tunnelling time. From the uncertainty principle, we know such a time, t_T, should be of order $\hbar$, but when using stationary states in a time independent potential, finding t_T is not so straightforward, indeed quite a controversy exists[8]. Our example suggested that one of these definitions, the extrapolated phase time[9] is not a good definition of tunnelling time as it stands. Unfortunately, we can shed no light on what is!

While we have only applied this method to a small range of examples[5], the results we have so far obtained are encouraging: the modifications seem to give quite different qualitative pictures for scattering. The esssential step forward from the Banks, Bender and Wu approach was to identify a general boundary between different WKB régimes. It can only be hoped that a similar generalisation of Coleman's field theoretic procedure[10] is possible.

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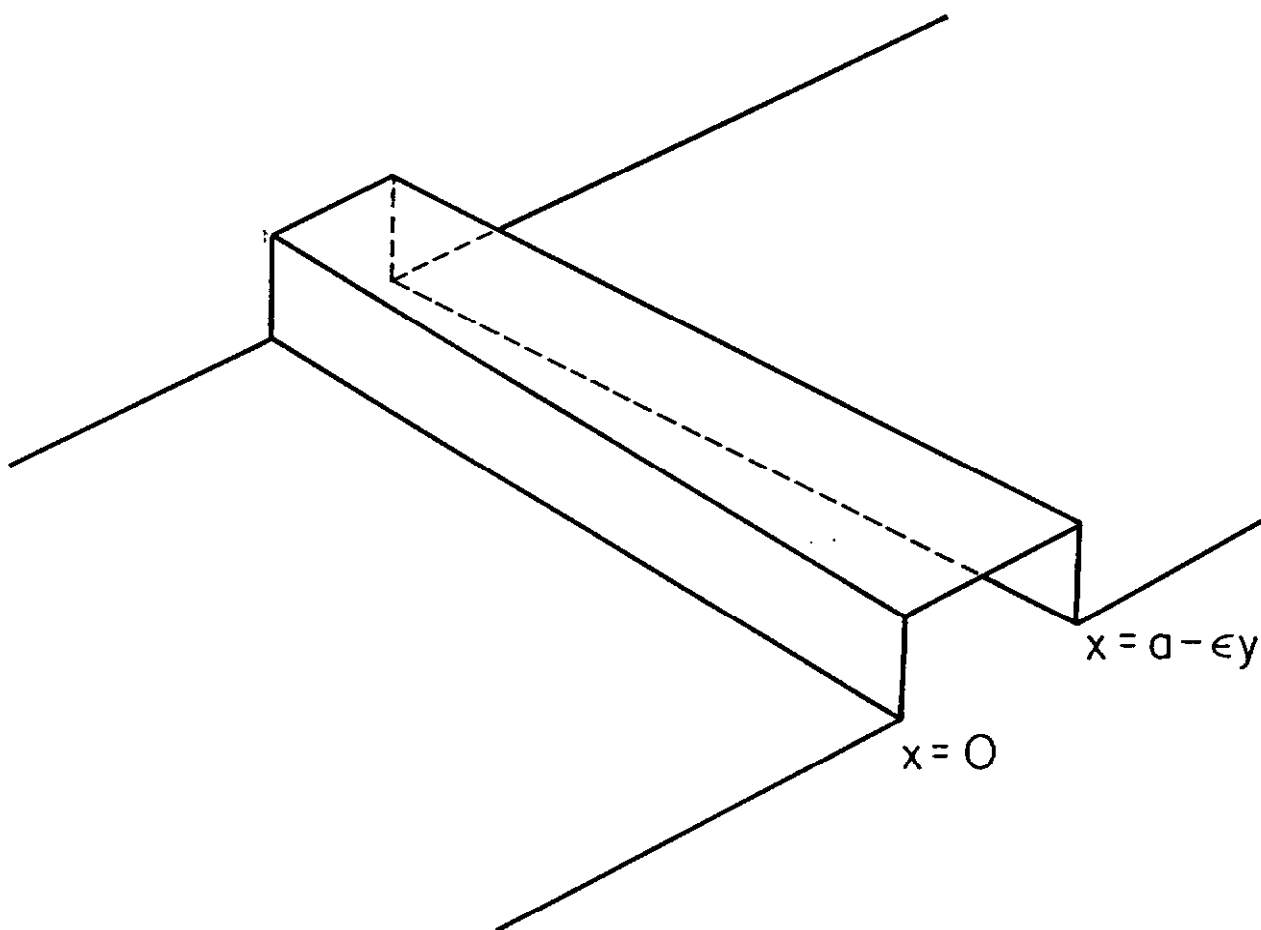**Figure 1.** The barrier $U(\mathbf{x}) = V\Theta(x)\Theta(a - x - \epsilon y)$.
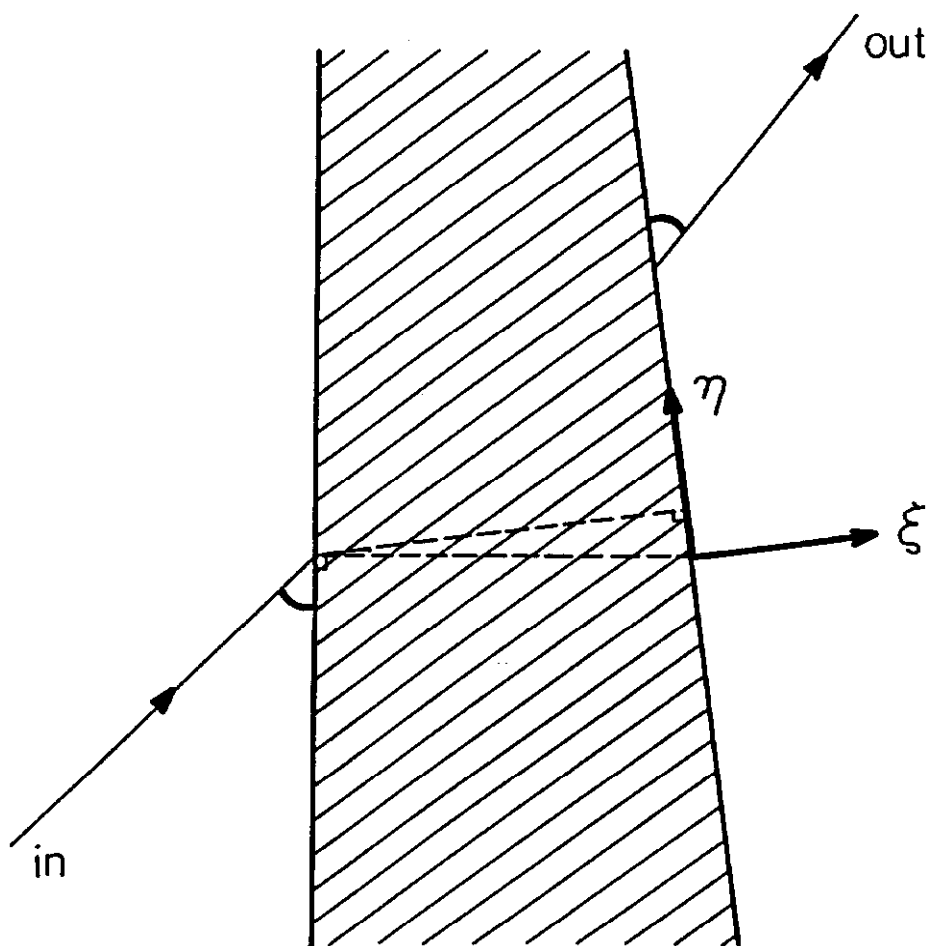
$x = a - \epsilon y$

$x = 0$

Figure 2. Trajectory of Gaussian peak scattering off barrier.